1-Pentanol

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.18e-11 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 8.95e-01

Confidence level: 9.61e-01

Nearest Neighbors from the Training Set

Image not found
1-Pentanol
Measured: 1.11e-11
Predicted: 1.18e-11

Image not found
Pentan-2-ol
Measured: 1.18e-11
Predicted: 1.20e-11

Image not found
3-Pentanol
Measured: 1.22e-11
Predicted: 1.20e-11

Image not found
Isopentyl alcohol
Measured: 1.31e-11
Predicted: 1.25e-11